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# Vibrational Excitations in Percolation: Localization and Multifractality

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# Vibrational Excitations in Percolation: Localization and Multifractality

## Abstract

We discuss localized excitations on the incipient infinite percolation cluster. Assuming a simple exponential decay of the amplitudes  $\psi_i$  in terms of the chemical (minimal) path, we show theoretically that the  $\psi$ 's are characterized by a logarithmically broad distribution, and display multifractal features as a function of the Euclidean distance. The moments of  $\psi_i$  exhibit novel crossover phenomena. Our numerical simulations of fractons exhibit a nontrivial distribution of localization lengths, even when the chemical distance is fixed. These results are explained via a generalization of the theory.

## Disciplines

Physics | Quantum Physics

## Vibrational Excitations in Percolation: Localization and Multifractality

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We discuss localized excitations on the incipient infinite percolation cluster. Assuming a simple exponential decay of the amplitudes  $\psi_i$  in terms of the chemical (minimal) path, we show theoretically that the  $\psi$ 's are characterized by a logarithmically broad distribution, and display multifractal features as a function of the Euclidean distance. The moments of  $\psi_i$  exhibit novel crossover phenomena. Our numerical simulations of fractons exhibit a nontrivial distribution of localization lengths, even when the chemical distance is fixed. These results are explained via a generalization of the theory.

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In recent years, it has been established that several physical quantities describing random systems do not obey the conventional scaling laws. Prominent examples are the growth probabilities of diffusion limited aggregation (for reviews see [1]), the voltage drops in random resistor networks [2], the energy dissipation in turbulence [3], the invariant measure of strange attractors in chaotic dynamical systems [4], and the probability density of random walks on random fractals [5]. All these quantities have a very broad distribution, and their moments cannot be described by a single exponent but an infinite hierarchy of exponents is needed to characterize them. This phenomenon is called multifractality and was first found in the context of turbulence [6].

Multifractality has also been discussed in the context of electron localization. At the mobility edge, separating localized and extended states, wave functions decay as power laws, and different moments of them (called inverse participation ratios) decay with exponents which are not trivially related to each other [7]. Below the mobility edge, the wave functions decay exponentially. For the one-dimensional Anderson model it is known that different moments of the wave functions decay with nontrivial powers of  $e^{-r}$  [3,8]. The resulting multifractal spectrum of exponents yielded a spectrum of correlation lengths. Not much is known about this spectrum for localized wave functions in other contexts.

In this Letter, we study localized states on disordered self-similar systems. As a specific example, we consider fractons on the infinite percolation cluster at criticality [9], which represents a standard model for such systems. Previously [10], we found that localized impurity states with energies  $E$  deep outside the band could be described by

$$\psi_i = \text{const} \times e^{-l_i/\lambda(E)}, \quad (1)$$

where  $l_i$  is the chemical distance (shortest path [11]) from the impurity at the origin to the point  $i$  and  $\lambda(E)$  is the localization length, measured along this chemical

path. In this Letter we show that the fact that  $l$  has a distribution of values for fixed Euclidean distance  $r$  results in a logarithmically broad, in fact multifractal, distribution of the moments  $\langle |\psi(r)|^q \rangle$ . However, in contrast to the usual multifractal case (but similar to the one-dimensional case treated by Paladin and Vulpiani in Refs. [3,8]), we find a critical ( $r$ -independent) value  $q_c$  above which  $\langle |\psi(r)|^q \rangle$  has the simple "unifractal" exponential behavior  $e^{-qr/\lambda}$ . In addition, we investigate the applicability of these results to localized vibrational excitations (fractons [12]), which have frequencies,  $\omega$ , inside the band. Our numerical data generally confirm the multifractal predictions but also indicate that Eq. (1) has to be generalized to allow  $\lambda$  to have a distribution of values for fixed  $l$  and  $\omega$ . Here we explore the simplest scenarios which are consistent with our numerical data.

Although we expect our results to apply to a large variety of localized states, it is convenient to discuss them in the specific framework of vibrational excitations on percolating clusters. These are approximated by the scalar equation of motion

$$\frac{d^2 u_i(t)}{dt^2} = \sum_{j=1}^N f_{ij} [u_j(t) - u_i(t)], \quad (2)$$

where  $u_i$  represents the displacement of the  $i$ th particle (of unit mass) from its equilibrium and  $f_{ij}$  are nearest-neighbor spring constants. Similar equations, with possible different diagonal terms involving  $u_i$  and  $du_i/dt$ , arise for spin waves, for random walks, and for electronic tight binding models [13]. Many of our results should also apply to these cases. The general solution of Eq. (2) can be expanded in terms of the eigenfunctions  $u_i(t) = A_i(\omega) \times e^{\pm i\omega t}$ , with eigenfrequencies  $\omega$ . In nonrandom lattices, the low-lying excitations are sound waves with wave vector  $q \sim \omega$ , and the amplitudes  $\psi_i(\omega) \equiv |A_i(\omega)|$  are spatially periodic functions. For random fractals, the low-lying vibrational modes are localized excitations (fractons). The "envelope" of these amplitudes decays with increasing distance from the center of the fracton, which

is taken at the site with the maximum amplitude, denoted  $\psi_0$ .

As discussed in Ref. [10], for energies  $E$  far from the band,  $\psi_i$  can be written as a sum of contributions over walks between the origin and site  $i$ . The sum is dominated by the minimal path, and Eq. (1) holds with a unique (one-dimensional) value  $\lambda(E)$ . In our context, this would imply that the moments of  $\psi_i$  at fixed  $l$  are trivial,

$$\psi_q(l, \omega) = \langle \psi_i^q(l, \omega) \rangle \sim \exp[-ql/\lambda(\omega)], \quad (3)$$

with a *single* localization length  $\lambda(\omega)$ . In what follows, we shall start by developing a full theory for the case when Eq. (3) holds. This theory certainly applies for deep impurity states, for localized states on topologically nonrandom one-dimensional chains (polymers, random walks), etc. We shall later discuss generalization of Eq. (3) as necessary. For convenience, we use the term "fracton" for any localized state. For a single fracton, we define

$$\psi_q(r, \omega) = \frac{1}{N_r} \sum_{i=1}^{N_r} \psi_i^q(r, \omega), \quad (4)$$

where  $N_r$  is the number of sites  $i$  at a distance  $r$  from the center of the fracton. If the sum in Eq. (4) contains  $N_l(r)$  sites which are at chemical distance  $l$  from the center, then we can write [14]

$$\begin{aligned} \psi_q(r, \omega) &= \frac{1}{N_r} \sum_l N_l(r) \left[ \frac{1}{N_l(r)} \sum_i \psi_i^q(l, \omega) \right] \\ &= \frac{1}{N_r} \sum_l N_l(r) \psi_q^{(r)}(l, \omega), \end{aligned} \quad (5)$$

where  $\psi_q^{(r)}(l, \omega)$  is the  $q$ th moment of  $\psi_i(l, \omega)$ , averaged over all sites  $i$  at fixed chemical distance  $l$  and radial distance  $r$ , for a single fracton. *A priori*, both  $\psi_q^{(r)}(l, \omega)$  and the fraction  $N_l(r)/N_r$  are random stochastic variables, which might depend on the specific fracton. However, assuming Eq. (3), we replace  $\psi_q^{(r)}(l, \omega)$  by  $\exp(-ql/\lambda)$ . Thus the fluctuations in  $\psi_q(r, \omega)$  result from those in  $N_l(r)/N_r$ . Averaging over *all* the possible realizations of percolation clusters, and replacing the sum in Eq. (5) by an integral, yields

$$\langle \psi_q(r, \omega) \rangle = \int_r^\infty \phi(l|r) \psi_q^{(r)}(l, \omega) dl, \quad (6)$$

where  $\phi(l|r)dl$  is the average of  $N_l(r)/N_r$  for a range  $dl$  near  $l$ . The normalized function  $\phi(l|r)$  is believed to be a scaling function of the variable  $r/l^{\tilde{\nu}}$ , for which a good approximation is [15,16]

$$\phi(l|r) = \frac{C_1}{l} \left[ \frac{r}{l^{\tilde{\nu}}} \right]^{\tilde{\delta}} \exp[-C_2(r/l^{\tilde{\nu}})^{\tilde{\delta}}], \quad (7)$$

for  $l > r$  and, of course,  $\phi(l|r) = 0$  for  $l < r$ . Here  $\tilde{\nu} = 1/d_{\min}$ , where  $d_{\min}$  describes the scaling of the average chemical (minimal) path,  $\langle l \rangle \sim r^{d_{\min}}$ , and  $\tilde{\delta} = (1 - \tilde{\nu})^{-1}$ . For fixed  $r$ ,  $\phi(l|r)$  has a maximum at  $l_{\max} = \alpha r^{d_{\min}}$ , with

$$\alpha = [\tilde{\nu} \delta C_2 / (\tilde{\nu} g + 1)]^{d_{\min} - 1}.$$

Inserting Eqs. (3) and (7) into Eq. (6), and using steepest descents, we find the saddle point at

$$l^* = \begin{cases} [\beta(q)]^{\tilde{\nu}-1} r & \text{for } r > r^*(q) \equiv \beta(q)^{-\tilde{\nu}} \alpha^{-\tilde{\nu} \tilde{\delta}}, \\ \alpha r^{d_{\min}} & \text{for } r < r^*(q), \end{cases} \quad (8a)$$

$$(8b)$$

where

$$\beta(q) = q/\lambda \tilde{\delta} \tilde{\nu} C_2 \equiv q/q_c. \quad (9)$$

The result of Eq. (8b) arises from the maximum in Eq. (7) itself,  $l^* = l_{\max}$ . Although it applies for *nonasymptotic* small values of  $r$ , it may dominate numerical data with finite values of  $r$  at small (viz., noninteger)  $q$ . Using Eqs. (8) and (9), we have

$$\ln \langle \psi_q(r, \omega) \rangle = \begin{cases} -C_2 \tilde{\delta} \beta(q)^{\tilde{\nu}} r & \text{for } r > r^*(q), \\ -(\alpha/\lambda) q r^{d_{\min}} & \text{for } r < r^*(q). \end{cases} \quad (10a)$$

$$(10b)$$

The steepest-descent result of Eq. (8) applies only for  $l^* > \lambda$  [17] and when  $l^*$  is in the integration range of Eq. (6),  $l^* > r$ , which implies that Eq. (10) holds only for  $\beta(q) < 1$ , i.e., when  $q < q_c$ . For  $q > q_c$ , the integral in Eq. (6) is dominated by its lower limit,  $l=r$ . As discussed in Ref. [10], we expect that  $\phi(r|r) \sim p^r \equiv \exp(-Cr)$  [18]. Thus,

$$\ln \langle \psi_q(r, \omega) \rangle = -[C + (q/\lambda)]r \text{ for } q > q_c. \quad (11)$$

For large  $r$ ,  $\langle \psi_q(r, \omega) \rangle$  obeys Eq. (10a) for  $q < q_c$  and Eq. (11) for  $q > q_c$ . Multifractality (in terms of the scale  $e^r$ ) shows up through the nonlinear dependence on  $q$  in Eq. (10a), which turns into a linear (unifractal) dependence for  $q > q_c$ . Equation (10a) could also be written as  $\langle \psi_q(r, \omega) \rangle \sim \exp(-\text{const} \times qr/\lambda_q)$ , with the unusually  $q$ -dependent localization length  $\lambda_q \sim q/\beta(q)^{\tilde{\nu}}$ .

Finally, we note that the multifractal behavior of Eq. (10a) is reflected in a logarithmically broad distribution function  $N(\ln \psi)$  of the amplitudes  $\psi_i(r, \omega)$  at fixed  $r$  and  $\omega$ : By inverting Eq. (1) one has  $l_i \equiv -\lambda \ln(\psi_i/\psi_0)$ , and  $N(\ln \psi)$  follows directly from  $\phi(l|r)$ , with  $l$  replaced by  $-\lambda \ln(\psi/\psi_0)$ .

Equations (10) and (11) summarize our theoretical predictions for an "annealed" average, which contains *all* possible configurations. As emphasized in Ref. [10], results will differ when one considers a single "typical" fracton. In that case, one would most probably encounter values of  $l$  near the peak of Eq. (7), i.e., with  $l \sim r^{d_{\min}}$ . Thus, we expect that

$$\ln[\psi_q(r, \omega)]_{\text{typ}} \propto -q r^{d_{\min}}/\lambda. \quad (12)$$

It is interesting to note that this result is the same as Eq. (10b): As  $q$  becomes small,  $\psi^q$  approaches  $1 + q \ln \psi$ . The value of  $\ln \psi$  is determined by the typical configurations. In fact, the "quenched" average  $\langle \ln \psi_i(r, \omega) \rangle$  scales as  $r^{d_{\min}}/\lambda$  for all values of  $r$  [10].

A simple example where our theory applies concerns an impurity state on a random walk. Here, Eq. (3) is exact,

Eq. (7) becomes a simple Gaussian, and our Eqs. (8)–(11) follow. Similar results apply for impurities on self-avoiding walks. The situation becomes more complicated when the underlying topological chain has some randomness. Such randomness implies some distribution of the values of  $\lambda(E)$  in Eq. (1). The averaging over  $\psi_l^q$  may thus yield a multifractal spectrum [3,8], replacing  $\psi_q^{(r)}(l, \omega)$  by  $\langle \psi_q(l, \omega) \rangle \sim \exp(-ql/\tilde{\lambda}_q)$ . Irrespective of the functional dependence of  $\tilde{\lambda}_q$ , we can still separate the average at fixed  $l$  from that over all  $l$ , and recover Eqs. (8)–(11) with  $\tilde{\lambda}_q$  replacing  $\lambda$  everywhere. This results in a more complicated  $q$  dependence of  $\langle \psi_q(l, \omega) \rangle$ . For a Gaussian distribution of the  $f_{ij}$ 's, one has [8]  $\beta(q) \sim q/\tilde{\lambda}_q \sim q + \mu q^2/2$ . For a *bounded* distribution,  $\beta(q)$  is bounded by a straight line, and one expects a crossover from the parabola to  $\tilde{\lambda}_q = \tilde{\lambda}_\infty$  for  $q$  larger than some threshold  $q^*$  of order unity [8].

To check if the predictions [and therefore also the assumption (3)] hold for states inside the band, we again return to the special example of fractons. We have performed extensive numerical simulations of fractons on critical 2D percolation clusters using the Williams-Maris technique [19], for  $\omega \approx 0.1$ . We first tested the assumptions leading to Eq. (3). We started by looking at the distributions of  $x \equiv l/|\ln[\psi_l(l, \omega)/\psi_0]|$  for single fractons. Equation (1) would imply a narrow distribution, centered around  $\lambda(\omega)$ . In practice, for the limited range of  $l < 200$  we had, we found distributions which were peaked around different values  $\lambda_s$  for different fractons  $s$ . Occasionally, these distributions had more than one peak, indicating different localization lengths for points reached via different paths. The average of  $\lambda_s$  over 50 fractons was of order  $20 \pm 2$ . The uncertainty in  $\lambda_s$  did not change significantly as  $l$  varied from 100 to 200.

Theoretically, the fluctuations in  $\lambda_s$  imply that we must replace Eq. (3) by

$$\psi_q^{(s)} = \int d\lambda p_s(\lambda, l) \exp(-ql/\lambda), \quad (13)$$

where  $p_s(\lambda, l)$  represents the distribution of  $\lambda$ 's for the fracton  $s$  and for points at a chemical distance  $l$ . The results for  $\langle \psi_q(r, \omega) \rangle$ , Eq. (6), would then require a double convolution, involving both  $\phi(l|r)$  and  $\langle p_s(\lambda, l) \rangle$ . Naturally, these results depend crucially on the average  $p(\lambda, l)$ , which is not known in our case. In the following we show that our numerical results are consistent with a  $\beta(q)$  crossing over to a straight line for  $q$  greater than unity, i.e., with a bounded distribution of the  $\lambda$ 's at fixed  $l$ .

The exponential factor in Eq. (13) emphasizes larger values of  $\lambda$  as  $ql$  increases, and therefore the results depend crucially on the tail of  $p_s$  for large  $\lambda$  and  $l$ . In our numerical studies, we evaluated the ratio  $-\ln[\psi_q^{(s)}(l, \omega)/\psi_q^{(s)}(0, \omega)]/ql$ . For each fracton, this ratio approached a constant value  $1/\lambda_s^x$  for  $ql > 200$ .  $\lambda_s^x$  may probably be identified with the largest value of  $\lambda$  in  $p_s(\lambda, l)$ . In practice,  $1/\lambda_s^x$  fluctuated among fractons, and the average

over 50 fractons gave  $\langle 1/\lambda_s^x \rangle \sim 0.035 \pm 0.002$ , or  $\lambda_s^x$  of about 29.

Assuming  $\psi_q^{(s)}(l, \omega) \sim \exp(-ql/\lambda_s^x)$ , we can now return to Eq. (6), and derive Eqs. (10) and (11), with  $\lambda_s^x$  replacing  $\lambda$ . Indeed, we calculated  $-\ln[\psi_q^{(s)}(r, \omega)/\psi_q^{(s)}(0, \omega)]/q\tilde{v}r$  for 50 fractons, and these numbers also approach plateaus for  $q\tilde{v}r \geq 100$ . The average of these values over 50 fractons was  $0.077 \pm 0.003$ . Using  $\lambda_s^x = 29$ ,  $\tilde{v} = 0.88$ ,  $g = 2.6$ , and  $C_2 \approx 1$  [15], we estimate that  $q_c = 213$ , so that all our data (with  $0.7 \leq q \leq 5$ ) are for  $q \ll q_c$ . Also,  $r^* \approx 50/q^{0.88}$ , so that Eq. (10a) should hold for  $q^{0.88}r > 50$ . Finally, Eq. (10a) yields  $\ln\langle \psi_q(r, \omega) \rangle \approx -0.075q^{0.88}r$ , which is in remarkably good agreement with the above numerical estimate.

It should be emphasized that in practical numerical simulations one is always limited to a finite number of configurations. For very large  $r$ , one would need an exponentially large number of attempts in order to probe the tail of  $\phi(l|r)$  for  $l \sim r$ . The annealed average done in Eq. (6), leading to Eq. (10), applies only for cases in which the sum in Eq. (4) actually contained points with  $l \sim l^*$ . This requires that  $N_r \phi(l^*|r) \geq 1$ . From Eq. (8a),  $l^* = 1.9r/q^{0.12}$ . Substitution into Eq. (7) then yields  $\phi(l^*|r) \sim \exp(-rq^{0.88}/110)$ . Since the number of points  $N_r$  at fixed  $r$  grows as a power of  $r$ ,  $N_r \phi(l^*|r)$  decays to zero for large  $r$ . Thus, for sufficiently large  $r$  we expect the annealed result to become irrelevant. Instead, the relatively small number of configurations will yield data with  $l$  near the peak of  $\phi$ , yielding the "typical" value of Eq. (12). In our simulations we had  $r < 100$ , so that  $N_r \phi(l^*|r)$  was not too small. Thus, at least some fractons should exhibit the annealed result of Eq. (10). This may explain the observed agreement between our data and Eq. (10). Combining Eq. (10) with this argument thus implies a gradual change from Eq. (10b), through Eq. (10a), to Eq. (12) [which has the same behavior of  $r^{d_{\min}}$  as Eq. (10b)]. Since the annealed result is expected only for an intermediate window, it may not be easy to observe in practice. We note that Lambert and Hughes [20] essentially averaged  $\ln \psi_i$ , and confirmed that  $\langle \ln \psi_i \rangle \sim r^{d_{\min}}$ , as in our Eq. (12), and as predicted previously [10]. In contrast, de Vries, de Raedt, and Lagendijk [21] essentially averaged over  $|\psi|^2$ , and found a simple exponential decay  $\langle |\psi|^2 \rangle \sim e^{-ar}$ , as in our Eq. (10a) or (11) and Ref. [10]. Such a result may be attributable to their limited range of  $r$ , as discussed above. One moral of the present discussion is that both  $l^*$  and  $r^*$  depend on  $q$ , so that one can change the borders of the above available range by looking at different moments.

In summary, we have shown that the amplitudes of vibrational eigenmodes on percolation clusters at criticality display novel multifractal features. More data at high  $q$  would thus be most welcome to check the predicted crossover for  $q > q_c$ . We have also shown that the distribution of  $\psi_l(l, \omega)$  exhibits some nontrivial features, which deserve further study. Particularly, our data indicate a finite maximal localization length  $\lambda_s^x$  on each fracton.

Assuming that this remains true, we obtained far-reaching conclusions concerning the multifractality of the wave functions. It would be very interesting to find out whether such an upper cutoff persists for larger values of  $l$ . Our theory can easily deal with more complicated situations, e.g., generalizations of Eq. (3) or of  $p_s(\lambda, l)$ .

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